\* This feff6 input file was generated by Artemis 0.8.012

\* Atoms written by and copyright (c) Bruce Ravel, 1998-2001

\* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

\* total mu\*x=1: 7.62 microns, unit edge step: 69.75 microns

\* specific gravity = 16.702

\* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

\* Normalization correction: 0.00030 ang^2

\* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \* -- \*

\* -----------------------------------------------------------------

\* The following crystallographic data were used:

\*

\* title ...

\* space = F m -3 m

\* a = 5.4640 b = 5.4640 c = 5.4640

\* alpha = 90.0 beta = 90.0 gamma = 90.0

\* core = U edge = L3

\* atoms

\* ! elem x y z tag occ

\* U 1.00000 1.00000 0.00000 U 1.00000

\* Ce 0.00000 0.00000 0.00000 Ce 1.00000

\* O 0.25000 0.25000 0.25000 O 1.00000

\* -----------------------------------------------------------------

TITLE ...

HOLE 4 1.0 \* U L3 edge (17166.0 eV), second number is S0^2

\* mphase,mpath,mfeff,mchi

CONTROL 1 1 1 1

PRINT 1 0 0 0

RMAX 6.0

\*CRITERIA curved plane

\*DEBYE temp debye-temp

NLEG 4

POTENTIALS

\* ipot Z element

0 92 U

1 92 U

2 8 O

ATOMS \* this list contains 75 atoms

\* x y z ipot tag distance

0.00000 0.00000 0.00000 0 U\_1 0.00000

1.36600 1.36600 1.36600 2 O\_1 2.36598

-1.36600 1.36600 1.36600 2 O\_1 2.36598

1.36600 -1.36600 1.36600 2 O\_1 2.36598

-1.36600 -1.36600 1.36600 2 O\_1 2.36598

1.36600 1.36600 -1.36600 2 O\_1 2.36598

-1.36600 1.36600 -1.36600 2 O\_1 2.36598

1.36600 -1.36600 -1.36600 2 O\_1 2.36598

-1.36600 -1.36600 -1.36600 2 O\_1 2.36598

2.73200 2.73200 0.00000 1 U\_2 3.86363

-2.73200 2.73200 0.00000 1 U\_2 3.86363

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4.09800 1.36600 1.36600 2 O\_2 4.53051

-4.09800 1.36600 1.36600 2 O\_2 4.53051

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-1.36600 4.09800 1.36600 2 O\_2 4.53051

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-1.36600 -1.36600 -4.09800 2 O\_2 4.53051

5.46400 0.00000 0.00000 1 U\_3 5.46400

-5.46400 0.00000 0.00000 1 U\_3 5.46400

0.00000 5.46400 0.00000 1 U\_3 5.46400

0.00000 -5.46400 0.00000 1 U\_3 5.46400

0.00000 0.00000 5.46400 1 U\_3 5.46400

0.00000 0.00000 -5.46400 1 U\_3 5.46400

4.09800 4.09800 1.36600 2 O\_3 5.95426

-4.09800 4.09800 1.36600 2 O\_3 5.95426

4.09800 -4.09800 1.36600 2 O\_3 5.95426

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END